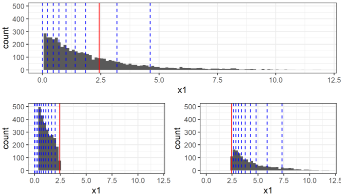
Introduction to Machine Learning

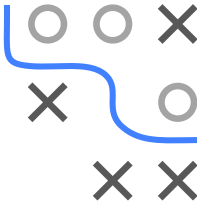
Gradient Boosting: Modern Techniques



Learning goals

- Know extensions of XGBoost and how they differ
- Understand areas upon which extensions of XGBoost improve

BEYOND XGBOOST



Next to **XGBoost** two other important modern boosting libraries exist:

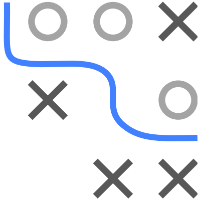
- **LightGBM** by **Ke et al. (2017)**
- **CatBoost** by **Prokhorenkova et al. (2017)**

Both libraries extend the ideas of **XGBoost** in several areas:

1. Tree growing efficiency
2. Data sampling
3. Feature compression
4. Categorical feature handling

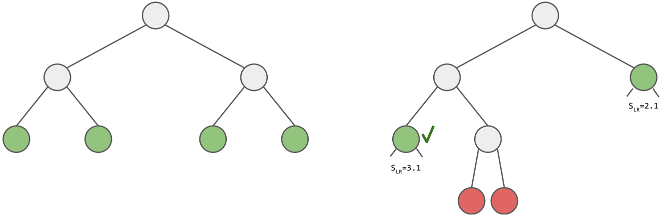
Many of the the proposed ideas have later been implemented in **XGBoost** as well.

TREE GROWING EFFICIENCY



Recall: **XGBoost** grows a balanced tree of `max_depth` and prunes leaves that do not improve the risk.

Leaf-wise (Best-first) Tree Growth allows the growing of unbalanced trees by comparing improvements between all possible leaves.



Balanced tree (left) of `max_depth`=3: All 4 leaves (colored green) will be split (in order from left to right). Leaf-wise growth (right) of `max_depth`=3: From the valid leaves (green), the leaf with largest improvement will be split next (marked). Invalid leaves (red) are not considered.

DATA SAMPLING: GRADIENT-BASED ONE-SIDE SAMPLING (GOSS)

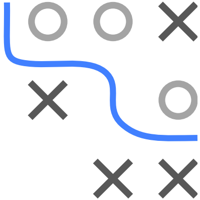
Recall: **XGBoost** use random data subsampling, i.e. stochastic gradient boosting.

Stochastic gradient boosting can be improved by *smarter* sampling strategies based on the values of the gradients.

GOSS:

- To evaluate a split GOSS only uses the $a \cdot n$ observations with largest (absolute) gradients and samples $b \cdot n$ observations from the remaining.
- The randomly sampled observations with smaller gradients are weighted by $\frac{1-a}{b}$.
- Default values are $a = 0.2$ and $b = 0.1$.
- GOSS is only used after $\frac{1}{\nu}$ iterations of regular boosting steps.

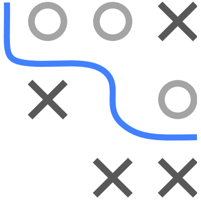
DATA SAMPLING: MINIMAL VARIANCE SAMPLING (MVS)



- MVS computes weights and selection probabilities of observations for a tree.
- The weighting is computed from the regularized absolute value $\hat{g}^{[m]}(\mathbf{x}^{(i)}) = \sqrt{g^{[m]}(\mathbf{x}^{(i)})^2 + \lambda h^{[m]}(\mathbf{x}^{(i)})^2}$.
- Observations with a value of $\hat{g}^{[m]}(\mathbf{x}^{(i)}) > \mu$ are always used and other observations are selected with probability $\frac{\hat{g}^{[m]}(\mathbf{x}^{(i)})}{\mu}$.
- μ has a closed-form nearly optimal solution for minimizing the risk of a tree base learner **(Ibragimov et al. 2019)**.
- For the tree fit each observation is weighted inversely proportional to its selection probability.

Note: $g^{[m]}(\mathbf{x}) = \frac{\partial L(y, f^{[m-1]}(\mathbf{x}))}{\partial f^{[m-1]}(\mathbf{x})}$ and $h^{[m]}(\mathbf{x}) = \frac{\partial^2 L(y, f^{[m-1]}(\mathbf{x}))}{\partial f^{[m-1]}(\mathbf{x})^2}$.

FEATURE COMPRESSION



For high dimensional (sparse) data it can be helpful to bundle similar features together to speed up split computations.

Exclusive feature bundling looks for mutually exclusive features, i.e. features that never take nonzero values simultaneously.

- A single histogram for approximate split finding in boosting can be built from multiple mutually exclusive features nearly without loss of information.
- Mutually exclusive features only occur in sparse data.
- This approach speeds up the histogram building from $\mathcal{O}(np)$ to $\mathcal{O}(nb)$ where b is the number of feature bundles.
- While finding the optimal bundling is *np*-hard, greedy approximations give good results empirically.

CATEGORICAL FEATURES

Even though **XGBoost** uses trees it does not support categorical features.

Both **LightGBM** and **CatBoost** provide *target* encoding strategies for categorical features:

$$\tilde{\mathbf{x}}_j = \frac{\sum_{i:\mathbf{x}_j = l} y^{(i)}}{N_l}, \quad l = 1, \dots, k$$

where N_l is the number of observations of the l'th level of categorical feature $\mathbf{x}_j$.

Additional noise can added to the encoding to avoid overfitting for level with few observations.

Features with relatively few levels $k \leq \tau_{\text{max\_cat\_to\_onehot}}$ (default 4) are one-hot encoded.

FEATURE COMPARISON OF BOOSTING FRAMEWORKS

	Parallel	GPU Support	Approx. splits	Categ. feats
XGBoost	*x*	*x*	*x*	
LightGBM	*x*	*x*	*x*	*x*
CatBoost	*x*	*x*	*x*	*x*
GBM				*x*
H2O	*x*	*x*	*x*	*x*
sklearn	*x*		*x*	*x*

	Tree growing		Subsampling		
			Observations		Feats
	Depth-wise	Leaf-wise	Regular	Gradient-based	
XGBoost	*x*	*x*	*x*	*x*	*x*
LightGBM	*x*	*x*	*x*	*x*	*x*
CatBoost	*x*	*x*	*x*	*x*	*x*
GBM		*x*	*x*		
H2O	*x*		*x*		*x*
sklearn	*x*		*x*		*x*